A33   Optimization of Thermal Chemistry Variables in Trace Explosives Detection

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After attending this presentation, attendees should have a better understanding of the complex chemistries that exist when studying explosive molecules alone and in mixtures in explosives trace detection.

This presentation will impact the forensic science community by providing a better understanding of the impact that thermal chemistry variables have on the maximum sensitivity of trace explosives.

The National Institute of Standards and Technology (NIST), Surface and Microanalysis Science Division, is working to build a chemical metrology program to support the widespread operational deployment and effective utilization of explosive trace detectors (ETD's) currently used throughout the United States for Homeland Security screening directives. The research goal is to optimize the detection of trace explosives by optimally manipulating the analytical conditions in the ETD's and thereby increasing the overall sensitivity of detection to potential threat compounds. There are many types of ETD's currently deployed in the United States, but the most common systems are based on ion mobility spectrometry (IMS). In a typical screening implementation, technicians swipe the surface of luggage, packages, cargo, etc. with a "trap" composed of cloth, paper, or Teflon coated materials. Traps are then introduced into the IMS instrument where the explosive particles are vaporized by rapid heating via a thermal desorber. The explosive vapor is then introduced into the ion source region where it is ionized using Beta emission from a ^{63}Ni source. After ionization, the analyte ions are injected into a drift tube where their atmospheric gas phase mobility is determined by their time of flight in a weak electric field. Ions traverse through the drift tube at different rates depending on their size, shape, and charge, and the resulting measured drift time is compared to a reference library of known explosives/narcotics for identification. Typically, thermal desorbers within ETD's are set to a relatively high temperature of 230-280 °C. This temperature range allows for the best chance of detection of a wide range of explosives (and narcotics) simultaneously. In this work, a series of experiments were conducted to optimize the desorber temperature for several common explosives based on 0.1-100 ng of deposited residues. By modifying the desorber temperature, order of magnitude increases in sensitivity were obtained for several high explosives. Optimal temperatures (giving the highest IMS sensitivity) were 60 °C for TNT, 100 °C for PETN, 140 °C for RDX, and 200 °C for HMX. These desorber temperatures are not in the typically used range noted above, and this data will be discussed in the context of developing optimized conditions for screening applications. Ongoing research is focused on developing similar optimization protocols for some of the more complex explosives such as plastic bonded explosives (C4, Semtex, and Detasheet) and ammonium nitrate fuel oil (ANFO). In addition, solution mixtures of the high explosives were analyzed to determine whether the enhanced sensitivity is also observed when multiple target analytes are present within a sample. Additional experiments designed to provide insights into the possible mechanisms of the observed sensitivity enhancements are also presented. These mechanisms include the concept that rather than vaporizing the sample in the desorber, there is liquid particle emission of the explosives. Preliminary studies indicate that upon rapid heating similar to that in ETD's, solid explosives desorb by first entering into a liquid phase before reaching gas phase equilibria.

During this process, aerosol emission via a bimodal distribution of droplet sizes was observed, including 100-200 nm droplets that egress into the vapor phase from the tops of droplets following a bursting of liquid-based bubbles and larger mm-sized droplets that emit from the desorption area after the droplet cavity collapses upon itself. The summation of presented data represents the complex chemistries that exist when studying explosive molecules alone and in mixtures. These detailed efforts may result in a better understanding of the chemical and physical processes involved in explosives trace detection.

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